

**POTENTIAL AND CURRENT CHARACTERISTICS OF LARGE AREA  
OLED USING NUMERICAL SIMULATION**

**PROJECT REPORT for SHA-798**

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**DECLARATION**

*I hereby declare that this submission '**Potential and Current characteristics of large area OLED using numerical simulation**' is a record of my project work carried out in the Unconventional electronics and photonics Laboratory of National Institute of Technology Calicut under the supervision of, Prof. P.Predeep, Dept. of physics, National Institute of Technology, Calicut and it is my own work and that, to the best of my knowledge and belief, it contains no materials previously published or written by another person, except where acknowledgement has been made in the text.*

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## ABSTRACT

Illumination of large area OLEDs is of great importance in the field of large area displays and solid state lightings. The major problem for large area OLED is the non homogeneous brightness due to non uniform distribution of current, in which the temperature is also have great influence on the current distribution. So it is relevant to find out the temperature distribution of large area OLED. In this work we are tried to get the temperature distribution of large area OLED using MATLAB programming. We got a non uniform current and potential distribution. The temperature distribution of  $5 \times 5 \text{cm}^2$  OLED is to be estimated using the finite element method (with MATLAB Programming). It will be non uniform [6] as shown in Fig 1. Non uniformity of light emission in large area OLED can be reduced by reinforcing the transparent electrode material with a metallic wire grid.

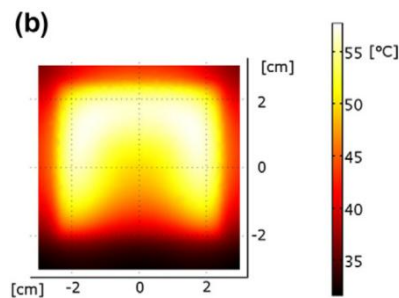


Fig (1) Temperature distribution in OLED [6]

## Contents

Chapter 1.....	7
1 Introduction.....	7
Chapter 2.....	8
2.1 Working and structure of OLEDs.....	8
2.2 Single layer OLED.....	11
2.3 Multi layer OLED.....	13
2.4 Efficiency of OLEDs.....	15
Chapter 3.....	16
3.1 Large area OLEDs.....	16
3.2 General challenges facing large area OLEDs.....	16
3.2.1 Non Homogeneity:.....	16
3.2.2 Power Supply:.....	17
3.2.3 Manufacturing problem (fabrication challenges).....	17
3.3 Potential distribution in OLED.....	18
3.4 Current distribution in OLED.....	19
3.5 Heat equation for OLED.....	19
Chapter 4.....	23
4.1 Numerical solution of potential and current equation using MATLAB.....	23
Chapter 5.....	25
5.1 Result and discussion.....	25
5.2 How to solve the problem.....	27
Conclusion.....	28
References.....	29

## Chapter 1

### 1 Introduction

Since the revolutionary invention of light bulbs by Thomas Edison in 1880s, electric lighting has been established as a standard technology. The technologies of fluorescent lamps and incandescent light bulbs are relatively mature and new scientific breakthroughs are not expected. Solid state lighting is a new environmentally friendly light source with potentially high efficiency. So far, light emitting diodes (LEDs) and organic LEDs (OLEDs) have been presented as candidates for SSL. Solid state lighting is a new environmentally friendly light source with potentially high efficiency [1].

The remarkable advance in OLEDs has led to its application to flat panel displays of high efficiency and has thus received a wide range of attention in recent years. Large area OLEDs is mainly used in Solid state lighting and flat-panel displays. Other remarkable advantage of OLEDs is the ability of color tuning due to the presence of numerous emitting materials in the visible range. Historically the electroluminescence (EL) of organic compounds was first demonstrated in 1953 by Bernanose. In 1987, a team (Tang and VanSlyke) in Kodak introduced a double layer organic light-emitting device (OLED) this OLED can be work in comparatively low voltage. In 2000 Shirakawa, Heeger and Mac Diarmid got Nobel Prize for the discovery of conducting polymers. In all this applications like solid state lighting flat-panel displays large area OLEDs have major role but the problem in large area OLEDs is non uniform distribution of current, temperature, and the light emitting from OLED. So we have to solve that problems, for solving, first we have to study the problem in details. In this paper mainly focusing on the non uniform temperature distribution in OLEDs

## Chapter 2

### 2.1 Working and structure of OLEDs

Carrier injection, transport, recombination and radiative exciton decay are the fundamental physical processes in OLED. Generally, if an external voltage is applied to the electrodes, electrons and holes are injected into the polymer. In the presence of an electric field the electrons and holes move through the active layer towards the oppositely charged electrode, approaching each other, upon meeting they form neutral excited states, called excitons. The injection of charge carriers into the polymer depends on the electronic energy structure of the active layer and on the work function of the metal electrodes.

When an electrical current is applied across the device, electrons are injected into the lowest unoccupied molecular orbital (LUMO) at the cathode to form radical anions and holes are injected into the highest occupied molecular orbital (HOMO) at the anode to form radical cations. These charge carriers migrate throughout the emissive layer under an electrical bias forming singlet and triplet excited states when oppositely charged species combine. The excited singlet state can relax radiatively and emit light (Figure 2) [2].

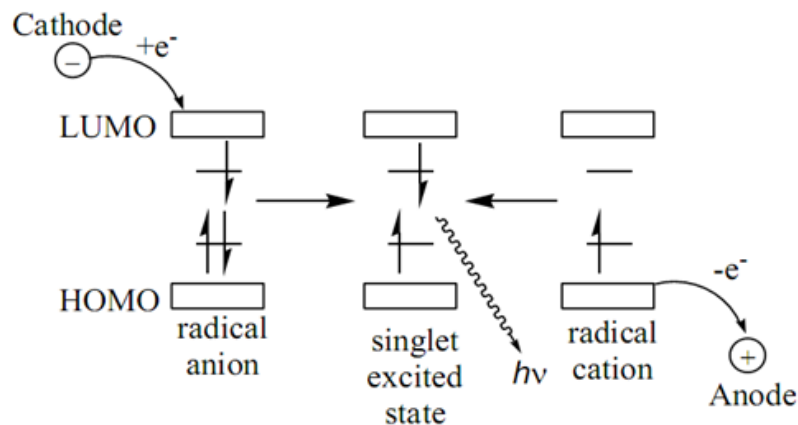


Fig 2: Radiative recombination of exciton.

In principle, an organic light emitting diode consists of a sequence of organic layers between two electrodes, an anode for hole and a cathode for electron injection, respectively. Schematically, the basic layers are assigned to the following functions (Figure 3):

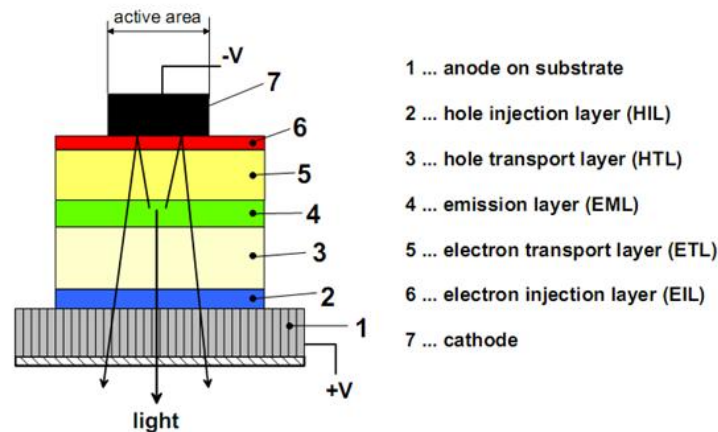


Fig: 3 Principle layer sequence of an OLED and the purpose of the layers.

Under positive bias, holes are injected from the anode and electrons from the cathode. The charge carriers drift through the transport layers and meet in the emission layer. There, they form excitons (neutral excited states or bound electron-hole pairs) which show a certain probability to decay radiatively. In order to achieve a high efficiency (emitted photons per injected electrons), the layers have to fulfill certain requirements. The hole injection layer (HIL) has to ease hole injection from the anode into the hole transport layer (HTL). This might be achieved by choosing the energetic level of the highest occupied molecular orbital (HOMO) to be in between the HOMO of the HTL and the ionization potential of the anode. For the simple picture given in Figure 4, the HOMO and LUMO levels are treated similar to valence and conduction bands in inorganic semiconductors and the vacuum level is assumed to be aligned. [3]



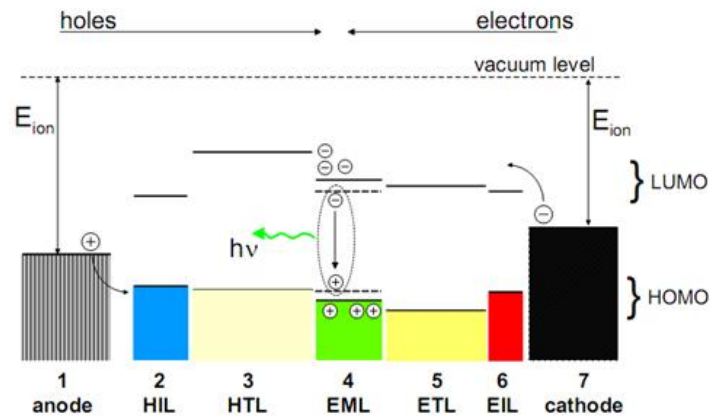


Fig: 4 Schematic view on a favorable energetic situation in an OLED.

The hole transport layer should have a high hole mobility and must hinder electrons coming from the cathode from reaching the anode. The properties of the electron transport (ETL) and electron injection (EIL) layers should be complementary to those of the HIL and HTL.

The cathode should be a low work-function metal like magnesium or calcium. Finally, at least one electrode must be transparent for visible light in order to achieve a high light out coupling efficiency. For that reason, in most cases, indium-tin-oxide (ITO) is used as transparent anode. Almost all realized OLEDs consists of fewer layers than proposed in Figure 3.

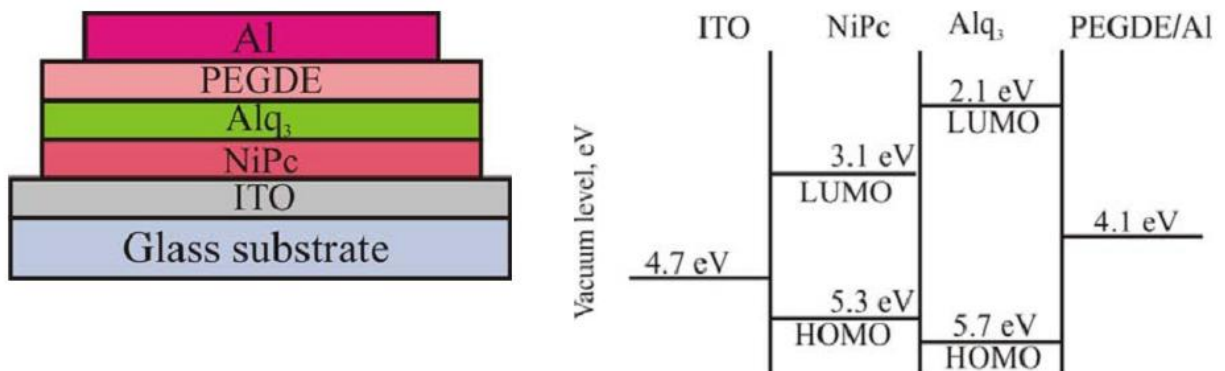


Fig: 5 Three layer OLED

This is due to the fact that some organic materials have combination of the properties mentioned above, for e.g. in fig 5 there are only two organic layers, a electron transport layer Alq3 and hole transport layer NiPc. The central layer fulfills all the qualities for an emission layer.

## 2.2 Single layer OLED

Single layer OLED have simple configurations and are industrially favorable because of its simple fabrication processes, less costly and time consuming. Thus, fabricating a single-layer device is very important and essential, in which the active organic material is capable of acting simultaneously as the hole transporting, electron transporting, light-emitting units quantum efficiencies.

To achieve efficient and long-lived single-layer devices, the active materials should satisfy several requirements: 1) desirable thermal stability and morphological properties in solid state, 2) satisfactory electrons and holes mobilities, and 3) appropriate energy levels for the highest occupied molecular orbital HOMO and the lowest unoccupied molecular orbital LUMO and high quantum efficiencies. A single-layer OLED can be fabricated from N,N-diphenylN,N-bis(1-naphthyl)1,1-biphenyl-4,4-diamine NPB, NPB has HOMO and LUMO of about 5.4 and 2.4 eV, respectively. poly(3,4-ethylenedioxythiophene):polystyrenesulphonic acid PEDOT:PSS, Ca, and Mg:Ag, are good electrodes for NPB [4]. For single layer OLED the one layer have lot of function so the operating voltage for single layer OLED will be very high and have a low lifetime.

The energies  $\Delta E_{h,e}$  required for hole and electron injection are determined by (i) the ionization potential  $I_p$  of the polymer, (ii) the electron affinity  $E_a$  of the polymer, and (iii) by the work-functions  $\Phi_{a,c}$  of the anode and cathode, respectively. The barrier to injection is determined according to the relations

$$\Delta E_h = I_p - \Phi_a \quad (2.2.1)$$

$$\Delta E_e = \Phi_c - E_a \quad (2.2.2)$$

To inject electrons into the polymer the cathode should be an electropositive metal with a low work-function close  $E_a$ , such as Al (4.3 eV), Mg (3.7 eV) or Ca (2.9 eV). For the injection of holes, the work-function of the anode should be close to  $I_p$ . Since one of the electrodes must be transparent for the observation of light-emission from the layer, usually an indium tin oxide (ITO) with a work function of 4.8–5.0 eV is used as the anode.

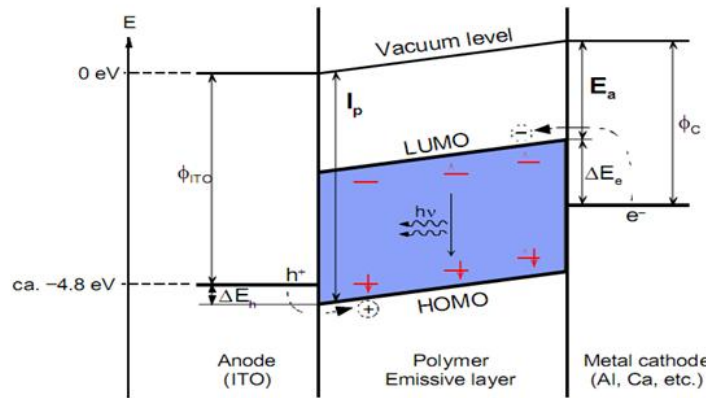


Fig: 6 Schematic energy level diagram for a single layer OLED

The recombination of electrons and holes in disordered organic materials obeys the Langevin law. In general, recombination is based on the concept that two oppositely charged carriers, which approach at a distance smaller than the Coulomb radius,  $r_C = e^2/4\pi\epsilon_r \epsilon_0 kT$ , will certainly recombine. Since the Coulomb radius in organic materials is significantly smaller than the layer thickness ( $r_C \sim 18$  nm at room temperature), a large density of injected carriers is necessary to enable efficient recombination of the carriers. For Langevin recombination, the recombination rate is determined by the approach of the carriers under their Coulomb attraction and the formation of the excitons, and thus, increases with the mobility of the charge carriers. Critical factors in constructing efficient EL devices are the barriers to hole and electron injection.

### 2.3 Multi layer OLED

The OLED performance (operating voltage, injection properties etc.) can be improved by using additional layers. Most organic semiconductors are better suited to transport holes rather than electrons, and recombination then takes place in the vicinity of the cathode. Recombination close to an electrode is generally predicted to be the case for unbalanced charge carrier concentration within the device, and the lifetime and efficiencies of the corresponding diodes are substantially decreased due to quenching effects. To overcome this problem, the recombination zone has to be shifted towards the center of the organic layer, and one approach is the fabrication of multi layer devices. The essential parameters for the device design and operation are the energy levels and the mobilities of holes and electrons of the respective layers.

The function of the additional layers is to serve (i) as blocking layers, i.e. to block charge carriers from traversing the device and reaching the other electrode without recombining, (ii) as injection or transport layers, i.e. enhancing either the injection or the transport of charge carriers. By means of appropriate design it is possible to enhance the recombination rate by balancing the charge carrier concentration, and to move the center of recombination away from the electrodes. In a basic two-layer OLED structure, one organic layer is specifically chosen to transport holes and the other organic layer is specifically chosen to transport electrons. The interface between the two layers provides an efficient site for the recombination of the injected hole–electron pair and resultant electroluminescence.

When an electrical potential difference is applied between the anode and the cathode such that the anode is at a more positive electrical potential with respect to the cathode, injection of holes occurs from the anode into the hole-transport layer (HTL), while electrons are injected from the cathode into the

electron-transport layer (ETL). The injected holes and electrons each migrate toward the oppositely charged electrode, and the recombination of electrons and holes occurs near the junction in the luminescent ETL. Upon recombination, energy is released as light,

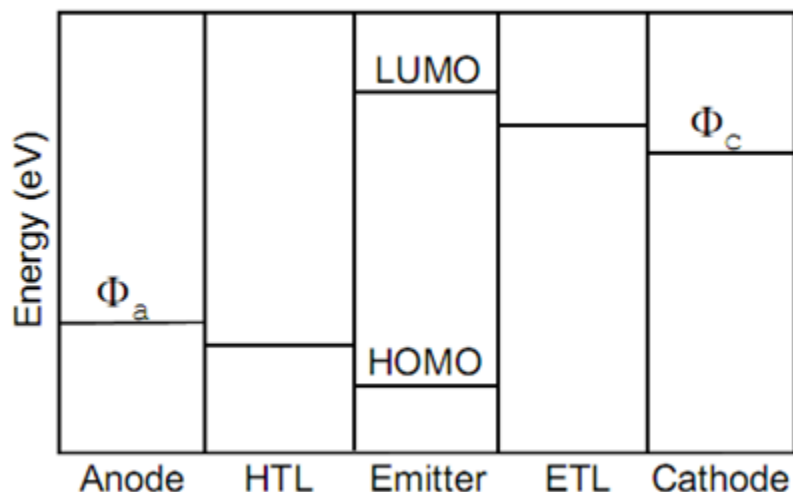


Fig: 7 Schematic energy level diagram for a multi layer OLED

As shown in Fig. 7, the highest occupied molecular orbital (HOMO) of the HTL is slightly above that of the ETL, so that holes can readily enter into the ETL, while the lowest unoccupied molecular orbital (LUMO) of the ETL is significantly below that of the HTL, so that electrons are confined in the ETL. The simple structure can be modified to a three-layer structure, in which an additional luminescent layer is introduced between the HTL and ETL to function primarily as the site for hole electron recombination and thus electroluminescence.

## 2.4 Efficiency of OLEDs

An expression of the internal EL quantum efficiency i.e. the number of generated photons per injected electron is given by:

$$\eta_{\text{int}} = \eta_{\text{PL}} \Phi_s \Phi_r \quad (3.1.1)$$

Where  $\Phi_s$  is the fraction of singlet state excitons formed, and  $\phi_r$  is the probability that charges recombine to excitons. In most organic materials,  $\Phi_s$  equal  $\frac{1}{4}$ . The parameter  $\phi_r$  is determined by the process of the injection of charge carriers and reaches the maximum of unity, if the current densities for injection of electrons and holes are equal. Thus, the maximum internal electroluminescence quantum efficiency in the case of an ideal electroluminescent device is 25 %.

Due to refraction, not all of the photons emitted can be perceived by an external observer. Therefore, the external quantum efficiency  $\eta_{\text{ext}}$  is defined as the number of photons actually leaving the device per injected electron, and  $\eta_{\text{ext}}$  is diminished by the factor of  $2n^2$  with respect to the internal efficiency

$$\eta_{\text{ext}} = \frac{\eta_{\text{int}}}{2n^2} \quad (3.1.2)$$

Where  $n$  is the refractive index of the organic layer. The maximum external quantum efficiency of any EL device is  $\sim 4\%$ :

$$\eta_{\text{ext}}(n=1.7) \leq 4\% \quad (3.1.3)$$

For the calculation of the luminance efficiency, the obtained luminance  $L$  is related to the current density  $j$  in the device:

$$\eta_{\text{lum}} = \frac{L}{j} \quad (3.1.4)$$

The unit of the luminous efficiency is candela per ampere (cd/A). Luminescence is directly proportional to the current densities.

## Chapter 3

### 3.1 Large area OLEDs

If the size (area) of OLEDs is greater than  $\text{cm}^2$  range it will be called as a large area OLED. Because of its large sizes it can be used for lighting large interior space, ceilings of a large hall. It has great applications In the case of displays for TVs and computers also.



Fig: 8 Large area OLED

### 3.2 General challenges facing large area OLEDs

#### 3.2.1 Non Homogeneity:

With increasing size of an OLED (area in the range of  $\text{cm}^2$ ) the light emission from the OLED will not be uniform. It is due to the non uniform distribution of the current. The temperature also non uniform because of this type of current distribution. This work is mainly focusing on this issue. This non uniformity is mainly due to the poor conductivity of the transparent electrode (anode) [5].

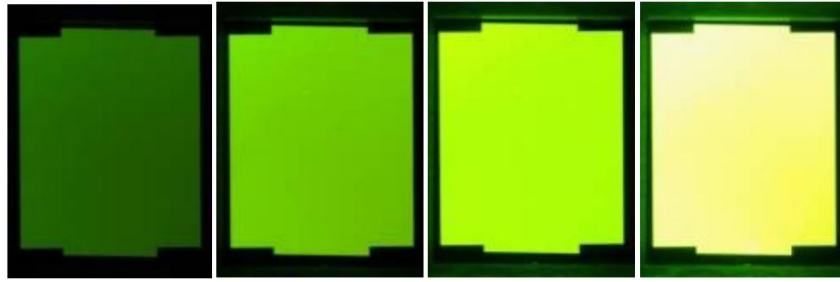


Fig: 9 Non Homogeneity in OLEDs [5]

Take about 12 points in OLED then Uniformity can be calculated by

Uniformity=minimum luminance among 12 points / maximum luminance among 12 points.

### 3.2.2 Power Supply:

Larger size OLEDs require larger currents, it is due to the limited conductivity of anode and larger area. So comparatively more power is needed for large area OLED.

### 3.2.3 Manufacturing problem (fabrication challenges)

Small defects in production or during operation can lead to device failure, with larger size the defect density has to be reduced dramatically.

Compare to all other challenges in the large area OLEDs, the main issue is non homogeneity, so it is much important to study on the potential, current and temperature distribution of large area OLEDs.



### 3.3 Potential distribution in OLED

Consider an OLED as a system of three conducting layers (anode organic layers and cathode). The thickness of the organic layer (100 – 250nm) is much smaller than lateral dimension; the connections are taken from the edges of anode and cathode. For calculating the potential following assumptions should be made

- 1) Lateral current densities (x- and y-direction) through the three layers are much higher than vertical currents (z-direction) along anode and cathode layers.
- 2) Current flow through organic layer between anode and cathode has only a vertical component (negative z-direction).[6]

$$J = -\sigma \text{ grad}\Phi \quad (3.3.1)$$

Where  $j$  is lateral current,  $\sigma$  is the electrical conductivity and  $\Phi$  is the potential distribution in the OLED.

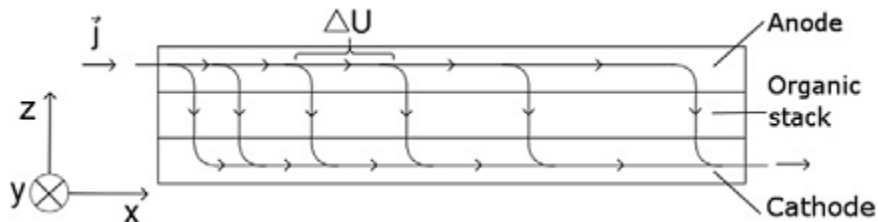


Fig: 10 Schematic representation of current flow in an OLED [6]

Vertical current (z direction)  $j_z$  can be written as [7]

$$\text{div}(d.J) = J_z \quad (3.3.2)$$

Substitute equation (3.3.1) in (3.3.2) which will give

$$d\sigma.\nabla^2(\Phi) = J_z \quad (3.3.3)$$

Sheet resistance of the electrode can be written as

$$R = 1/(d\sigma) \quad (3.3.4)$$

Boundary conditions are

- a)  $\Phi = \Phi_{\text{applied}}$  at the boundaries of electrode which are connected with a voltage source.
- b)  $\text{Grad}(\Phi).n = 0$  at the boundaries of electrode which are not connected to the voltage source. Where  $n$  is the normal to the electrode boundary.

By solving the equation (3.3.3) with appropriate boundary condition we can get the potential distribution of OLED

### 3.4 Current distribution in OLED

In case of large area OLED, current distribution measurement is of great importance. By substituting the solution of potential equation (3.3.3), the current distribution in large area OLEDs is given by

$$J = -\sigma \text{grad}\Phi \quad (3.4.1)$$

### 3.5 Heat equation for OLED

Consider an OLED kept in air. The temperature of air with respect to OLED is called ambient temperature let it be  $T_{\text{amp}}$ . OLED is kept in air, there

will be a temperature gradient between OLED and air. The conduction heat rate perpendicular to each of the control surface at the  $x$ ,  $y$ ,  $z$  co-ordinates are represented by  $q_x$ ,  $q_y$ ,  $q_z$  respectively. Then the conduction heat at the opposite surface can be expressed as a Taylor series and it is given by [8]

$$q_{x+dx} = q_x + \left(\frac{\partial q_x}{\partial x}\right) dx \quad (3.5.1)$$

$$q_{y+dy} = q_y + \left(\frac{\partial q_y}{\partial y}\right) dy \quad (3.5.2)$$

$$q_{z+dz} = q_z + \left(\frac{\partial q_z}{\partial z}\right) dz \quad (3.5.3)$$

Within the medium there will be a source term associated with the rate of thermal energy generation which can be represented as

$$E_g = q dx dy dz \quad (3.5.4)$$

Where  $q$  is the rate at which energy is generated per unit volume of the medium.

The energy storage inside the medium can be represented as

$$E_{st} = \rho C_p \frac{\partial T}{\partial t} dx dy dz \quad (3.5.5)$$

Physically  $E_{st}$  represent the rate of change of thermal energy stored by the mater.

According to the conservation of energy the energy stored inside the medium can be represented as

$$E_{st} = E_{in} + E_g - E_{out} \quad (3.5.6)$$

Where  $E_{in}$  is the heat flow towards the medium  $E_g$  is the energy storage term,  $E_{out}$  is the heat flow out of the medium. Substitute equation (3.5.4) and (3.5.5) in equation (3.5.6)

$$q_x + q_y + q_z + q dx dy dz - q_{x+dx} - q_{y+dy} - q_{z+dz} = \rho C_p \frac{\partial T}{\partial t} dx dy dz \quad (3.5.7)$$

Substitute from equation (4.5.1), (4.5.2), and (4.5.3), the equation (4.5.7) becomes

$$-\left(\frac{\partial q_x}{\partial x}\right) dx - \left(\frac{\partial q_y}{\partial y}\right) dy - \left(\frac{\partial q_z}{\partial z}\right) dz + q dx dy dz = \rho C_p \frac{\partial T}{\partial t} dx dy dz \quad (3.5.8)$$

The conduction heat rate may be evaluated from Fourier's law

$$q_x = -k dy dz \frac{\partial T}{\partial x} \quad (3.5.9)$$

$$q_y = -k dx dz \frac{\partial T}{\partial y} \quad (3.5.10)$$

$$q_z = -k dx dy \frac{\partial T}{\partial z} \quad (3.5.11)$$

Substitute equation (3.5.9), (3.5.10), and (3.5.11) into equation (3.5.8) and dividing out the dimensions of control volume (dx dy dz), we get

$$\frac{\partial}{\partial x} \left( \frac{k \partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{k \partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{k \partial T}{\partial z} \right) + q = \rho C_p \frac{\partial T}{\partial t} \quad (3.5.12)$$

For convenience substitute Q instead of q and rearranging, the equation (3.5.12) can be written as

$$\rho C_p \frac{\partial T}{\partial t} + \text{div} (-k \text{ grad} T) = Q \quad (3.5.13)$$

where  $\rho$  is the material density  $C_p$  as specific heat capacitance, 'k' is specific heat conductivity and Q as heat source. This equation is called Heat equation.

For the interfaces between the device and ambient, boundary conditions for exchange of heat by convection and radiation are calculated with the following equation

$$n(-k \text{ grad} T) = h(T - T_{\text{amb}}) + \epsilon \sigma (T^4 - T_{\text{amb}}^4) \quad (3.5.14)$$

Where  $n$  is the normal vector to the boundary  $h$  as heat transfer coefficient,  $\epsilon$  as emissivity,  $\sigma$  as Stefan Boltzmann constant and  $T_{amb}$  as ambient temperature.

The first term in the right side of equation (3.5.14) is due to the heat transfer by convection and this expression is coming from Newton's Law of Cooling. This term depends on the conditions in the boundary. Here the value of  $h$  is taken as 5 and ambient temperature is 298 K.

The second term in the right side of equation (3.4.14) is coming due to the radiation transfer of heat energy from the surface of the device. This will depends on the surface area of the device. Mathematically that term is expressed by Stefan-Boltzmann Law.

In the Heat equation  $Q$  is the heat source. This heat is produced due to the current passing through the device i.e. Joule heating. Thus  $Q$  will be depends on the electric field and the current it can be written as

$$Q = p = E.J \quad (3.5.15)$$

Where  $p$  is the total power density of the device. It is the sum of the electrical losses in electrode, and the organic layer

$$p = p_{org} + p_{electrode} \quad (3.5.16)$$

These power densities can be calculated as

$$p_{org} = (j_z)^2 / \sigma_{org} \quad (3.5.17)$$

$$p_{electrode} = \frac{1}{dR} \times (\text{grad}\Phi)^2 \quad (3.5.18)$$

Substitute this power terms as heat source in equation (3.5.13) then this equation can be solve with Finite Element Method.

## Chapter 4

### 4.1 Numerical solution of potential and current equation using MATLAB

In MATLAB there is a tool called ‘PDE tool’ which can be used to solve the partial differential equation. This PDE tool contains many type of inbuilt partial differential equation like Poisons equation, Laplace equation, Heat equation, diffusion equation etc.

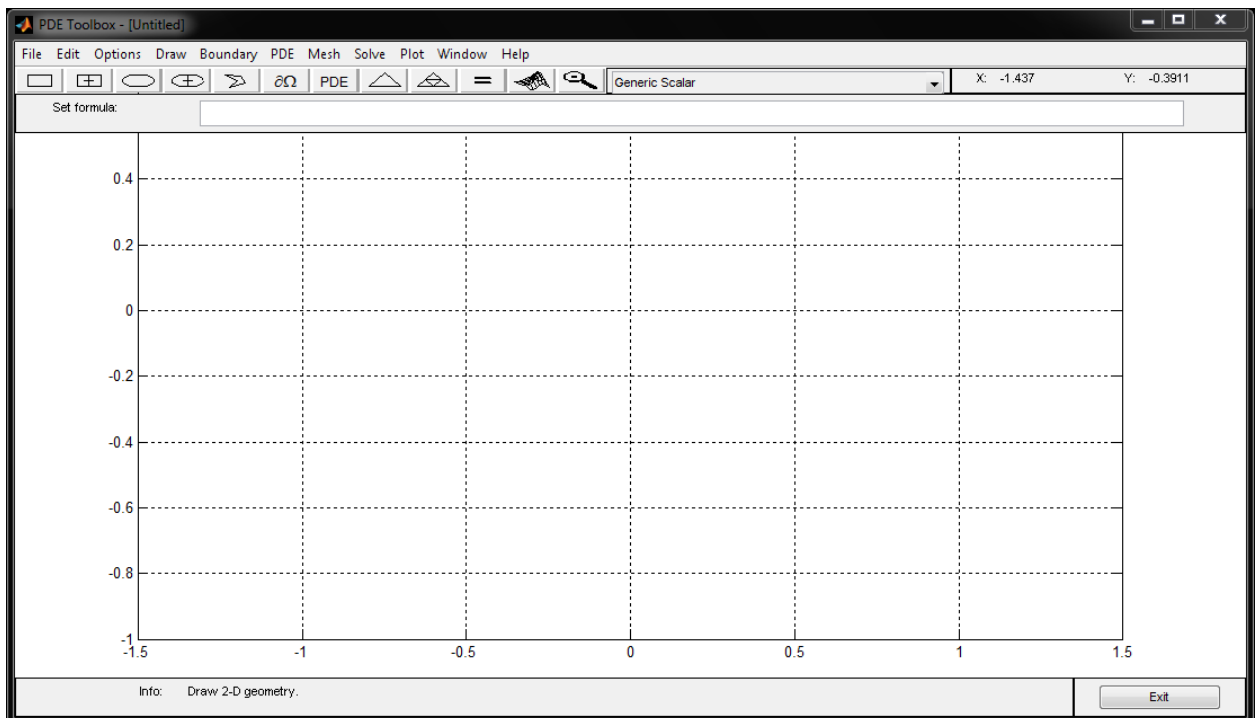


Fig: 11 PDE tool box in MATLAB

The potential equation is in the form of Poisson’s equation and it is given by

$$\nabla^2(\Phi) = j_z R$$

Where  $\Phi$  is the potential distribution and R is sheet resistance.

Assume homogeneous current of 300mA and sheet resistance of  $0.3\Omega/\square$ . And substitute these values in the above equation. The PDE tool contains the similar equation, so the values can be substitute simply. First draw the

rectangular box then take the boundary condition option in the PDE tool; substitute the boundary condition as discussed above (put maximum applied voltage (5.4V) in the boundary which is connected to the voltage source). Mesh should be generated after drawing the rectangular box. After substituting the necessary values and boundary conditions we can adjust the X and Y axes limits and grid spacing, let it be 0.1 then go to solve PDE section thus we can solve the PDE equation. The output will be in the form of plots either in 2D or 3D. This plot will give the distribution of the potential. Any directional view can be made by rotating this plot.

## Chapter 5

### 5.1 Result and discussion

After solving the potential and current distribution equation numerically with the help of MATLAB programming, the Potential distribution and current distribution profile in OLED is shown in fig 12 and fig 13.

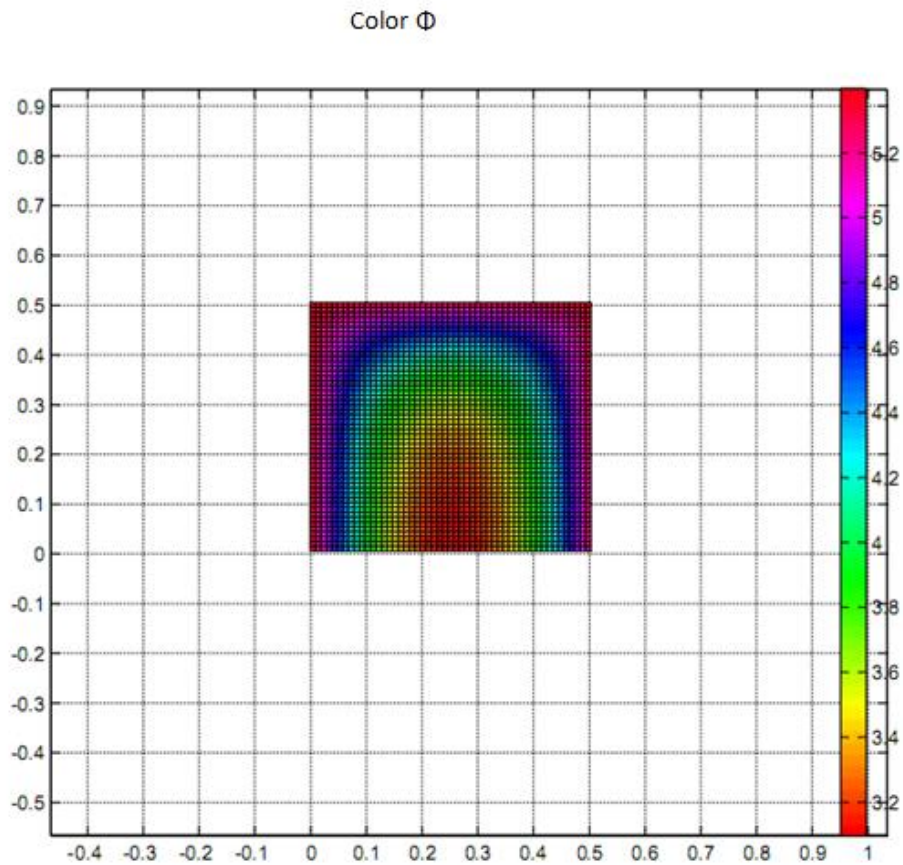


Fig: 12 Potential distribution in OLED



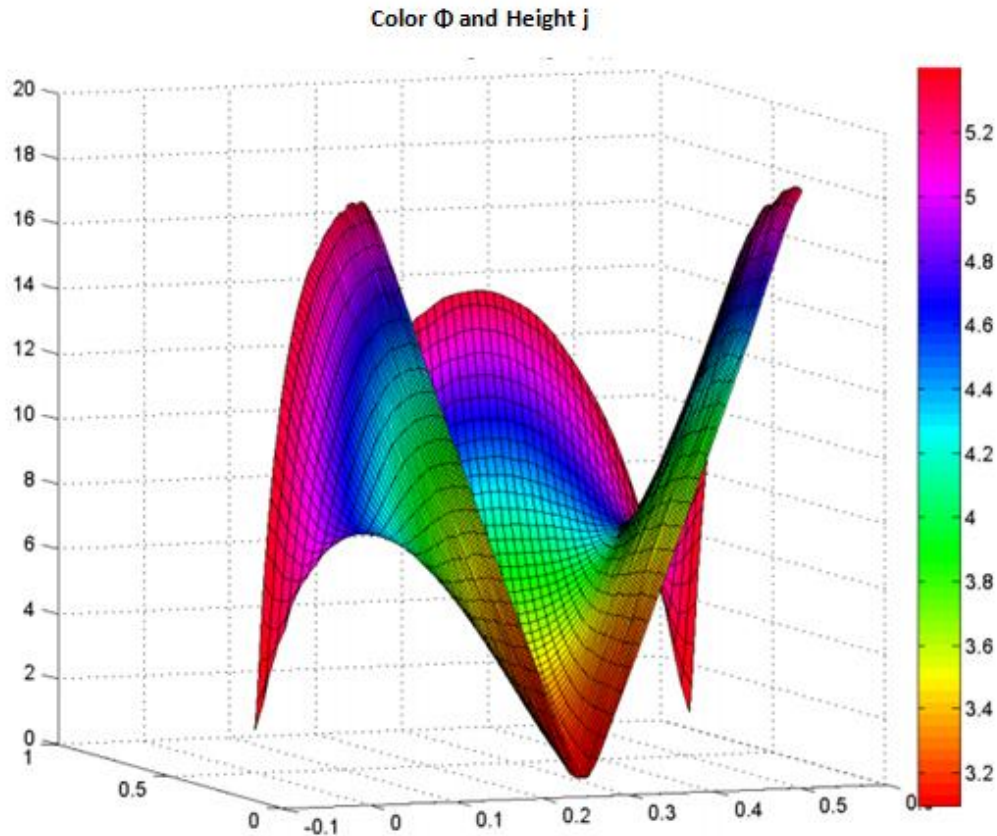


Fig: 13 Potential and current distribution.

Fig: 12 describe potential distribution alone (color represent the potential distribution), maximum potential distribution is in the top edge. Next maximum potential distribution is in the top side edges. In fig: 13 both potential and current distributions are there. Current is maximum in the two side edges. Most minimum current is in the lower edge. This both figure gives a non uniform potential and current distribution. From this potential and current distribution the Heat equation can be solved using Finite element Method, thus finally we will get the temperature profile. According to equation (3.1.4) luminescence is proportional to current distribution hence luminescence is also non uniform.

## 5.2 How to solve the problem

The resistivity of the transparent electrode will lead to an appreciable lateral voltage drop if the lateral current flow reaches a certain value. The luminance of the OLED depends on the voltage over the organic layers and may also become inhomogeneous. The conductivity of the electrode material and the size of the pixel play an important role in this inhomogeneity. These inhomogeneities can be reduced by reinforcing the transparent electrode material with a metallic wire grid. Indium-tin-oxide (ITO) was replaced with a conductive polymer electrode and an electroplated thick metal grid was used to improve the homogeneity of the potential distribution over the transparent polymer electrode [5] By integrating metal grids with polymer electrodes, the luminance increases more than 24% at 6 V and 45% at 7 V compared to the polymer electrode devices without a metal grid. This implies that a lower voltage can be applied to achieve the same luminance, hence lowering the power consumption. Furthermore, metal grid integrated OLEDs exhibited less variation in light emission compared to devices without a metal grid.

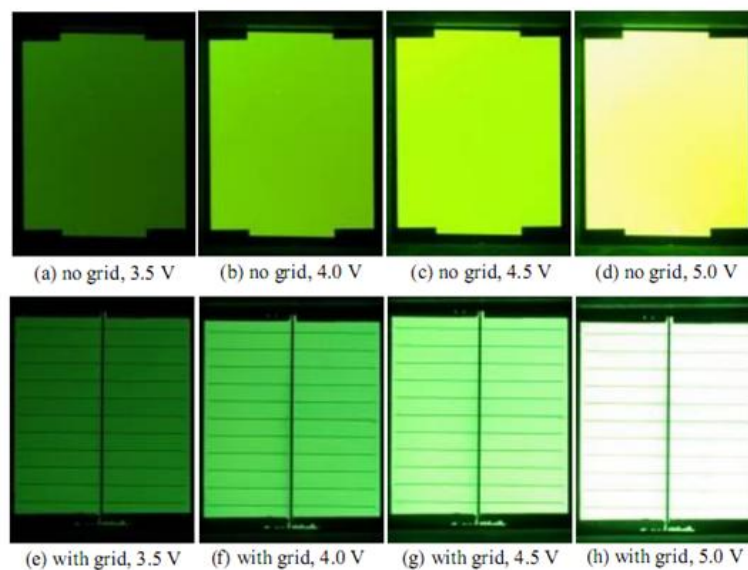


Fig: 14 (a)-(d) ITO free large area OLED without a metal grid. (e)-(h) ITO free large area OLED with a grid[5]

The current first flows through the low-resistance auxiliary metal lines to the central region and then diffuses into ITO, producing highly homogeneous light over a large area. In addition, the current density (luminous intensity) over a large area is expected to increase.

## **Conclusion**

In the case of large area OLEDs current, potential and temperature distribution is non uniform. Final result of this non uniform distribution is the inhomogeneous light emission. So this is a major problem in large area OLED. Any research activities for reducing this problem are of great importance.

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